

Why rooting fails

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Why rooting fails

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I explore the origins of the unphysical predictions from rooted staggered fermion algorithms. Before rooting, the exact chiral symmetry of staggered fermions is a flavored symmetry among the four "tastes." The rooting procedure averages over tastes of different chiralities. This averaging forbids the appearance of the correct 't Hooft vertex for the target theory.

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1. Introduction

My presentation [1] at last year's meeting in this series discussed what were some of the unphysical consequences arise from the rooting prescription usually used along with the staggered quark formalism. In particular, I showed how an excess symmetry leads to an incorrect quark mass dependence. That argument is elucidated somewhat further in [2, 3]. Here I explore this problem more deeply to understand why these wrong predictions appear. In particular, I will demonstrate that a strong mixing of tastes with different chiralities leads to an incorrect 't Hooft vertex.

The outline is as follows. In section 2 I summarize the naive arguments in favor of the rooting trick. This includes treating of the determinant as a sum over loops and empirical observations on the eigenvalues of the Dirac operator on typical gauge configurations. Section 3 reviews the basic formulation of staggered fermions and how the rooting is implemented. Section 4 turns to some issues related to chiral symmetry that signal caution. In particular, the method involves an averaging over fermion chiralities. Also, on moving between topological sectors, the taste symmetry of the eigenvalue spectrum must break. In section 5 I connect these issues to an old topic, the "'t Hooft vertex." Here I show how symmetries forbid the rooting procedure from correctly reproducing the requisite form. Section 6 raises a few questions, hinting at why the approximation may not be too bad for the two light plus one intermediate mass situation. I also suggest some possible ways to repair the algorithm. Section 7 briefly states the final conclusion that rooting can often be a good approximation but predictions for non-perturbative physics where the 't Hooft vertex is important can not be trusted.

2. Naive justifications for rooting

The basic argument for rooting comes from consideration of the fermion contribution as a determinant of the Dirac operator. A determinant is a sum over permutations of the rows of the matrix. Each permutation in turn is a product of cycles. Each cycle represents a fermion loop in perturbation theory. Now with unrooted staggered fermions on a smooth gauge field background, we have an excess in the number of species by a factor of four. Thus each loop is counted four times too much. By replacing the determinant with its fourth root, this effectively multiplies each loop by a factor of one quarter, giving exactly the desired contribution from a single fermion. The conclusion is that the rooting procedure does give the correct perturbative expansion. As a special case, rooting is correct for the continuum limit of the free fermion theory as well.

This argument relies on symmetry between the four "tastes" of the unrooted theory. The importance of this is strongly emphasized in Ref. [4]. Numerical evidence for the required symmetry appears in studies of the eigenvalues of the Dirac operator; for example, Ref. [5], shows that as the lattice spacing becomes small the eigenvalues tend to group into approximately degenerate quartets. Rooting effectively selects one eigenvalue from each quartet.

These arguments for rooting are further supported by the rather spectacular successes of recent simulations. Indeed, a variety of observables that had previously been calculated in the "valance approximation" have now been redetermined with dynamical quarks treated using the fourth root approximation. The agreement with experiment is uniformly much better with the dynamical quarks included. For example, see Ref. [6].

Unfortunately these arguments have seduced many into suggesting that the algorithm might become exact in the continuum limit, i.e. that the lattice artifacts might go away as the lattice spacing is taken to zero [7]. The purpose of this talk is to provide a proof that this is impossible; there exist certain important physical effects that the algorithm inherently must miss.

3. Staggered review

To proceed I need to delve into the heart of the staggered algorithm. For this I begin with the so called “naive” discretization of the Dirac equation. This considers fermions hopping between nearest neighbor lattice sites while picking up a factor of $\pm i\gamma_\mu$ for a hop in direction $\pm\mu$. Going to momentum space, the discretization replaces powers of momentum with trigonometric functions, for example

$$\gamma_\mu p_\mu \rightarrow \gamma_\mu \frac{\sin(ap_\mu)}{a}. \quad (3.1)$$

Here I denote the lattice spacing by a . This formulation exposes the famous “doubling” issue, arising because the fermion propagator has poles not only for small momentum, but also whenever any component of the momentum is at π/a . The theory represents not one fermion, but sixteen.

It is important to note that the various doublers have differing chiral properties. This arises from the simple observation that

$$\frac{d}{dp} \sin(p)|_{p=\pi} = -\frac{d}{dp} \sin(p)|_{p=0}. \quad (3.2)$$

The consequence is that the helicity projectors $(1 \pm \gamma_5)/2$ for a travelling particle depend on which doubler one is observing.

Now consider a fermion traversing a closed loop on the lattice. As shown in Fig. 1, the corresponding gamma matrix factors will always involve an even number of any particular γ_μ . Thus the resulting product is proportional to the identity. If a fermion starts in a single spinor component, it will wind up in the same component after circumnavigating the loop. The determinant exactly factorizes into four equivalent pieces. The naive theory has an exact $U(4)$ symmetry, as pointed out some time ago by Karsten and Smit [8]. Indeed, for massless fermions this is actually a $U(4) \otimes U(4)$ chiral symmetry. This symmetry does not contradict any anomalies since it is not the full naive $U(16) \otimes U(16)$ of 16 species. The chiral symmetry generated by γ_5 remains exact, but this is allowed because it is actually a flavored chiral symmetry. As mentioned above the helicity projectors for the various doubler species use different signs for γ_5 .

The basic idea of staggered fermions is to divide out this $U(4)$ symmetry [9, 10, 11] by projecting out a single component of the fermion spinor on each site. Taking $\psi \rightarrow P\psi$, one projector that accomplishes this is

$$P = \frac{1}{4} \left(1 + i\gamma_1 \gamma_2 (-1)^{x_1+x_2} + i\gamma_3 \gamma_4 (-1)^{x_3+x_4} + \gamma_5 (-1)^{x_1+x_2+x_3+x_4} \right) \quad (3.3)$$

where the x_i are the integer coordinates of the respective lattice sites. This immediately reduces the doubling from a factor of sixteen to four.

At this stage the naive $U(1)$ axial symmetry remains. Indeed, the projector used above commutes with γ_5 . This symmetry is allowed since four species, usually called “tastes,” remain. Among

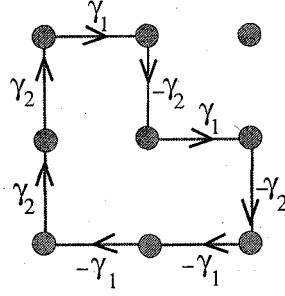


Figure 1: When a fermion circumnavigates a loop in the naive formulation, it picks up a factor that always involves an even power of any particular gamma matrix.

them the symmetry is a taste non-singlet; under a chiral rotation, two rotate one way and two the other.

The next step taken by most of the groups using staggered fermions is the rooting trick. In the hope of reducing the multiplicity down from four, the determinant is replaced with its fourth root, $|D| \rightarrow |D|^{1/4}$. With several physical flavors this trick is applied separately to each. As argued in the previous section, in simple perturbation theory each fermion loop gets multiplied by one quarter, cancelling the extra factor from the four “tastes.”

At this point one should be extremely uneasy: the exact chiral symmetry is waving a huge red flag. Symmetries of the determinant survive rooting, and thus the exact $U(1)$ axial symmetry for the massless theory remains. For the unrooted theory this was a flavored chiral symmetry. But, having reduced the theory to one flavor, how can there be a flavored symmetry without multiple flavors?

At this point I need to make a somewhat technical comment on chiral symmetry. It is usually regarded in terms of an $SU(N_f) \otimes SU(N_f)$ symmetry for the massless N_f flavor theory. This is believed to be spontaneously broken, and, via the Goldstone mechanism, explains the lightness of the pions. However, this is also a symmetry of the **massive** theory regarded in terms of its parameter space. More specifically, consider a mass term of form

$$\frac{1}{2}(\bar{\psi}_L M \psi_R + \bar{\psi}_R M^\dagger \psi_L) \quad (3.4)$$

where M is a complex N_f by N_f matrix. Then physics is invariant under changing the mass parameters

$$M \rightarrow g_L^\dagger M g_R. \quad (3.5)$$

Here g_L and g_R are arbitrary matrices in $SU(N_f)$.

In this context it is important to note that the theory is **not** invariant under a simple phase change $M \rightarrow e^{i\theta} M$. Such a rotation is anomalous and changes the strong CP violating angle. This is the reason there are only $N_f^2 - 1$, rather than N_f , Goldstone bosons. In the particular case of one flavor QCD, there should be no surviving chiral symmetry whatever. That theory is expected to be analytic in the fermion mass in the vicinity of the origin [12]. Unfortunately, a phase change in the mass term is an exact symmetry of the staggered fermion determinant and remains so on rooting. This incorrect behavior was the main subject of my discussion last year [1].

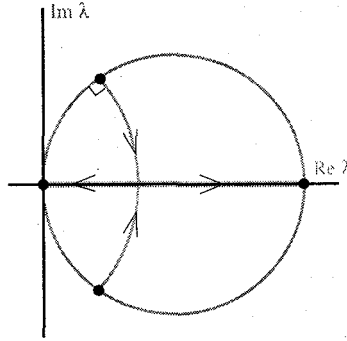


Figure 2: In the overlap formulation a single exact zero eigenmode is possible. In transiting from winding number zero to one, a pair of complex eigenvalues disappear and are replaced with the exact zero mode and a compensating mode on the opposite side of the overlap circle.

4. Where things go awry

So the rooted theory appears to have some issues related to chiral symmetry and the anomaly. Before rooting, the one exact chiral symmetry is actually a non-singlet symmetry because the different tastes are associated with different gamma matrix conventions. Thus there are two tastes of each chirality. What happens to this symmetry on rooting?

Consider the index theorem for a gauge configuration with unit winding. Near the continuum limit there should be one approximate zero mode for each of the tastes. These are not exact zero modes because of finite spacing effects, but that is not the issue here. Because the tastes differ in chirality, two of these modes will be left handed and two right handed in the sense of the physical helicity projectors for the corresponding fermions. What rooting does is average over these. While this allows the chiral symmetry to remain, it does not correspond to the single chirality mode of the target theory. The issue is analogous to trying to make a living organism out of a racemic mixture of proteins; it won't work.

Note that the staggered projection operator in Eq. 3.3 satisfies

$$P\gamma_5 = \gamma_5 P = (-1)^{x_1+x_2+x_3+x_4} P. \quad (4.1)$$

This means that the oscillating factor $(-1)^{x_1+x_2+x_3+x_4}$ plays the role of γ_5 . This matrix is independent of gauge configuration and as such remains traceless independent of the gauge field winding number. This is another way to see that the approximate zero modes must come in opposite chiralities.

This behavior is unlike that with other formulations. In usual “continuum” discussions, the appearance of zero modes is compensated by modes that move in from infinity. With Wilson fermions the chiral zero modes are paired with heavy doubler states. With the overlap operator [13], a zero mode has a compensating mode occurring on the opposite side of the overlap circle. This behavior with the overlap is sketched in Fig. 2, taken from my Lattice '02 presentation [14]. The overlap formulation introduces a modified chirality matrix $\hat{\gamma}_5$ which does depend on the gauge fields. The winding number is given by the relation $v = \text{Tr } \hat{\gamma}_5 / 2$.

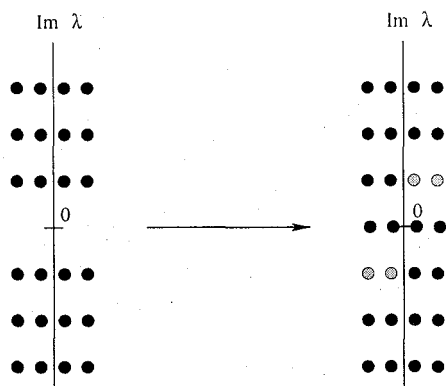


Figure 3: In transiting between different winding number sectors, the clustering of the staggered Dirac eigenvalues into taste quartets must break down.

The approximate zero modes have implications for how the staggered eigenvalues must evolve as one moves between topological sectors. For a smooth gauge field with zero winding number, near the continuum limit there is numerical evidence that the Dirac eigenvalues indeed cluster into taste quartets. A similar structure is desired with smooth gauge fields carrying a unit of winding, although in this case there should be one quartet of approximate zero modes. However on considering rough gauge fields that interpolate between these situations, the quartets must necessarily break apart. In particular, two of the approximate zero modes must drop down from above in the complex eigenvalue plane, while two rise up from below. This necessarily leaves a mismatch in the form of “holes” that must be absorbed in the non-zero eigenvalue spectrum, as sketched in Fig. 3.

Note that, despite claims to the contrary [4], this chiral mixing has nothing to do with the order of taking the continuum limit and going to zero mass. Even when the mass remains finite, a topologically non-trivial gauge configuration should still generate fermion eigenvalues with approximately zero imaginary part. The mass merely gives these modes a finite real part. I do, of course, assume that the lattice spacing is small enough that the chiral modes corresponding to topology are clearly identifiable.

5. The 't Hooft vertex

So the concerns with rooting involve zero modes of the massless Dirac operator. Through the index theorem, this in turn is tied to the topological structure of the gauge field. To explore the consequences of this connection, start with the usual integration of the fermionic fields in terms of determinant of the Dirac operator, D . For any given configuration of gauge fields, this determinant is the product of the eigenvalues of this matrix. To control infrared issues, insert a small mass and write the resulting path integral

$$Z = \int dA e^{-S_g} \prod_i (\lambda_i + m). \quad (5.1)$$

Here the λ_i are the eigenvalues of the kinetic part of the fermion determinant and S_g is the pure gauge part of the action. On taking the mass to zero, any configurations which contain a zero

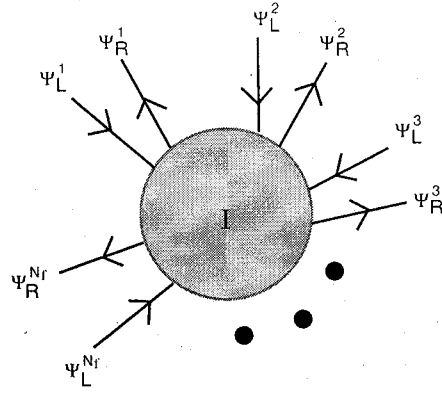


Figure 4: With N_f flavors the 't Hooft vertex is a $2N_f$ fermion interaction where each flavor flips its spin.

eigenmode will have zero weight in the path integral. This suggests that for the massless theory one can ignore any instanton effects since the corresponding configurations don't contribute to the path integral. Does this mean that "instantons" are irrelevant in the continuum limit?

Indeed, 't Hooft [15, 16] pointed out long ago why this conclusion is incorrect. The issue is not whether the zero modes contribute to the path integral, but whether they can contribute to physical correlation functions. To see how this goes, add some sources to the path integral

$$Z(\eta, \bar{\eta}) = \int dA d\psi d\bar{\psi} e^{-S_g + \bar{\psi}(D+m)\psi + \bar{\eta}\eta + \eta\bar{\psi}}. \quad (5.2)$$

Differentiation (in the Grassmann sense) with respect to η and $\bar{\eta}$ gives any desired fermionic correlation function. Now integrate out the fermions

$$Z = \int dA e^{-S_g - \bar{\eta}(D+m)^{-1}\eta} \prod_i (\lambda_i + m). \quad (5.3)$$

Consider a source that overlaps with an eigenvector of D corresponding to one of the zero modes, i.e.

$$(\psi_0, \eta) \neq 0. \quad (5.4)$$

The source contribution introduces a $1/m$ factor into the path integral. This cancels the m from the determinant, leaving a finite contribution as m goes to zero.

With multiple flavors, the determinant will have a mass factor from each. When several masses are taken to zero together, one will need a similar factor from the sources for each. This product of source terms is the famous "'t Hooft vertex." [15, 16] While it is correct that instantons do drop out of Z , they survive in correlation functions.

So, with N_f flavors the theory generates a $2N_f$ -fermion effective interaction, as sketched in Fig. 4. This is a purely non-perturbative phenomenon. In this interaction, all flavors flip their spin, and this forms the basis of the anomaly. With several flavors this is a high dimensional operator, but it remains relevant since the high dimensions are compensated by powers of the strong interaction scale, Λ_{qcd} . Indeed, the resulting interaction is non-local at this scale.

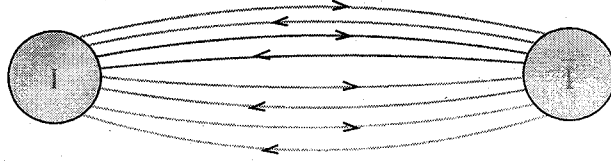


Figure 5: In calculating the instanton/anti-instanton interaction, a contribution will arise from the exchange of all tastes. This introduces an unphysical singularity in the rooted theory.

For the unrooted staggered theory with its four tastes, the expected 't Hooft vertex is an octilinear interaction $\sim (\bar{\psi}\psi)^4$. It strongly couples all the tastes, even in the continuum limit. It does not violate the exact chiral symmetry of the theory because it involves two tastes of each chirality.

Now for the target one flavor theory, the 't Hooft vertex should reduce to a simple bilinear interaction $\sim \bar{\psi}\psi$. This has the form of a mass shift and is inconsistent with any exact chiral symmetry, including that of the unrooted theory. Indeed, that symmetry forbids the generation of such a term in the rooted theory. The absence of this vertex in the rooted approximation has serious consequences; in particular, the rooted theory will have an incorrect renormalization group flow for the fermion mass.

One might try to argue that since the unrooted determinant goes as the mass to the fourth power, the rooted formula goes only linearly in the mass. Then to cancel the zero only requires one taste source. So why not just measure the vertex for one taste and ignore the others?

Unfortunately this will not work. The basic vertex strongly couples all tastes. In the unrooted theory the strength of this coupling scales as the product of m^{-4} from the sources times m^4 from the determinant. This leaves a mass independent contribution. However the rooted theory still has the m^{-4} factor from the sources but only $(m^4)^{1/4} \sim m$ from the rooted determinant. Thus the rooted vertex displays a m^{-3} singularity at vanishing mass. The scale of this singularity is set by Λ_{qcd} and there is no lattice spacing suppression. Note also that high gluon momenta are not involved, unlike the taste mixing arising in perturbation theory.

Because of this strong coupling between the tastes, all four must be considered in intermediate states. This will give unphysical contributions to quantities such as multi-instanton interactions. To be more explicit, imagine trying to calculate a correlation function of two pseudo-scalar glue-ball operators $F\tilde{F}(x)$ and $F\tilde{F}(y)$. This will receive a contribution from instanton/anti-instanton pairs. That, in turn, will have a contribution from the exchange of all four tastes, as sketched in Fig. 5. In the unrooted theory the contribution of this diagram scales as the mass to the zeroth power and has a spatial dependence arising from the overlap of the approximate fermion zero modes of the two topological objects. On rooting the determinant factors associated with the instantons have a reduced mass dependence, leaving behind a m^{-6} mass dependence for this correlation. This is dramatically different from the desired target one flavor theory, where the exchange of the single physical fermion scales again as a mass independent constant. Note that for the physical case the exchange of four copies of the fermion in the zero mode is forbidden by the Pauli principle.

6. Questions

Several open questions remain on the rooting procedure. Would a square root of the determi-

nant be better? In particular, the doublers do occur in equivalent pairs. Also the reduction from four to two flavors should leave behind a residual chiral symmetry; so, the exact symmetry is not in itself necessarily bad. The detailed form of the 't Hooft vertex will still couple the extra tastes, but this might be a small effect.

Are these issues all associated with light quarks and could the wrong chiral behavior of the rooting become unimportant for massive quarks? Indeed, if this is the case and the square root is also a better approximation, then the numerical successes of staggered fermions for the two light plus one intermediate mass quark case would be easier to understand.

Can counter-terms fix things? One might try to add a counter-term to mimic the desired 't Hooft vertex and another to cancel the unphysical singularity. This would require some tuning of the strengths of the counter-terms. Also, given the non-local nature of the 't Hooft vertex, it is unclear whether these terms would have to be non-local. But perhaps this would be an acceptable price to pay for the gained efficiency of the staggered approach.

Instead of rooting, it might be possible to cancel the extra tastes with bosonic ghosts. To avoid the unphysical averaging over chiralities, this would require a chiral formulation for the ghosts. But since they are bosonic, this might not impose the computational costs of directly simulating chiral fermions.

7. Conclusion

The conclusions of this discussion are quite succinctly stated. First, rooting is a justified perturbative procedure. As such, it can be accurate for many physical quantities. However it cannot become exact in the continuum limit because it does not generate the correct 't Hooft vertex. This makes the scheme particularly dangerous for the treatment of non-perturbative physics in singlet channels.

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